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MATHEMATICAL METHODS IN COORDINATION CHEMISTRY: TOPOLOGICAL·

AND GRAPH-THEORETICAL IDEAS IN THE STUDY OF METAL CLUSTERS·

AND POLYHEDRAL ISOMERIZATIONS

by

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MATHEMATICAL METHODS IN COORDINATION CHEMISTRY: TOPOLOGICAL AND GRAPH-THEORETICAL IDEAS IN THE STUDY OF METAL CLUSTERS AND POLYHEDRAL ISOMERIZATIONS

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Abstract

Mathematical ideas taken from disciplines such as topology and graph theory provide new insights into key areas of coordination chemistry such as structure and bonding of metal clusters as well as polyhedral isomerizations.

A-1

Introduction

An area of increasing importance during the past several decades has been coordination chemistry, namely the chemistry of compounds containing central metal atoms surrounded by donor ligands of various types. Coordination compounds play major roles in diverse areas of practical importance ranging from molecular catalysis to solid state devices and metal ions in biological systems. The scientific and practical importance of coordination chemistry is indicated by large and regular international conferences on coordination chemistry since 1952.

In recent years one of the specific interests in my group at the University of Georgia has been the development of new mathematical methods for understanding chemical structure, bonding, and reactivity with particular emphasis on approaches using the mathematical disciplines of topology, graph theory, and group theory. This paper presents an overview of such work in the two areas of metal cluster bonding topology and polyhedral isomerizations. Both of these areas are of considerable interest to coordination chemists.

This paper is based on a lecture given at the most recent international conference on coordination chemistry, which was held in Athens, Greece, in August, 1986.[1] Because of space limitations only a general view of the key ideas can be presented here. Readers wishing further details are directed to the cited references for additional information.

Metal Cluster Bonding Topology

In 1977 Rouvray and I[2] first published a novel approach to metal cluster structure and bonding based on ideas taken from graph theory. Subsequent experience indicates the following strengths for this method:

(1)   The ability to deduce important information about the electron counts and shapes of diverse metal clusters using a minimum of computation.

(2) The ability to generate reasonable electron-precise bonding models for metal clusters that appear intractable by other methods not requiring heavy computation.

(3) Information concerning the distribution of total metal cluster electron counts between skeletal bonding within the cluster polyhedron and bonding to external ligands.

(4) Ability to distinguish between localized and delocalized bonding in metal cluster polyhedra.

Metal clusters treated effectively by this approach include post-transition metal clusters,[3] osmium carbonyl clusters,[4] gold clusters,[5,6] platinum carbonyl clusters,[5,7] and rhodium carbonyl clusters having fused polyhedra.[8,9]

In our approach the topology of chemical bonding can be represented by a graph in which the vertices correspond to atoms or orbitals participating in the bonding and the edges correspond to bonding relationships. The adjacency matrix $\underset{\sim}{A}$ of any graph, including a graph representing chemical bonding as above, can be defined as follows:

$$A_{ij} = \begin{cases} 0 \text{ if } i = j \\ 1 \text{ if } i \text{ and } j \text{ are connected by an edge} \\ 0 \text{ if } i \text{ and } j \text{ are not connected by an edge} \end{cases} \qquad (1)$$

The eigenvalues of the adjacency matrix $\underset{\sim}{A}$ are obtained from the following determinantal equation:

$$|\underset{\sim}{A} - x\underset{\sim}{I}| = 0 \qquad (2)$$

where $\underset{\sim}{I}$ is the unit matrix ($I_{ii} = 1$ and $I_{ij} = 0$ for $i \neq j$).

These eigenvalues x relate to the Hückel theory molecular orbital energies E and the Hückel parameters α and β by the following equation[2]:

$$E = \frac{\alpha + x\beta}{1 + xS} \qquad (3)$$

Positive and negative eigenvalues x thus correspond to bonding and antibonding orbitals, respectively.

The atoms at the vertices of a metal clusters can be classified as light atoms or heavy atoms. A light atom such as boron or carbon uses only its s and p orbitals for chemical bonding and therefore has 4 valence orbitals (sp^3) which require 8 electrons for a stable closed shell spherical bonding manifold (i.e., the Lewis octet rule). A heavy atom such as a transition metal or post-transition metal uses s, p, and d orbitals for chemical bonding and therefore has 9 valence orbitals (sp^3d^5) which require 18 electrons for a stable closed shell spherical bonding manifold (i.e., the stable 18-electron configurations of most transition metal carbonyl derivatives). The valence orbitals of the vertex atoms are partitioned into internal orbitals involved in the skeletal bonding of the cluster polygon or polyhedron and external orbitals involved in bonding to external groups or ligands such as monovalent external groups (e.g., hydrogen, halogen, alkyl, aryl) in the case of light atom vertices and carbonyl groups, tertiary phosphines, cyclopentadienyl, benzene, lone electron pairs, etc., in the case of transition metal heavy atom vertices.

The two extreme types of chemical bonding in metal clusters may be called edge-localized and globally delocalized.[2,10] An edge-localized polyhedron has two-electron two-center bonds along each edge of the polyhedron and is favored when the numbers of internal orbitals of the vertex atoms match the numbers of edges meeting at the corresponding vertices (i.e., the vertex degree). Since vertex atoms in metal clusters normally use three internal orbitals for cluster bonding, cluster polyhedra exhibiting pure edge-localized bonding normally have only degree three vertices (e.g., the tetrahedron, cube, or various prisms). A globally delocalized polyhedron has a multicenter core bond in the center of the polyhedron and is formed when the numbers of internal orbitals do not match the vertex degrees. Intermediate degrees of delocalization may occur in sufficiently large or complicated polyhedral networks.

An important achievement of the graph-theory derived approach to the bonding topology in globally delocalized systems is the demonstration of the close analogy between the bonding in two-dimensional planar polygonal aromatic systems such as benzene and that in three-dimensional boranes and carboranes based on deltahedra without tetrahedral chambers.[2,9,10] In this context a _deltahedron_ is defined to be a polyhedron in which all faces are triangles (Figure 1). In both the two-dimensional and three-dimensional systems the three internal orbitals from each vertex atom are partitioned into two twin internal orbitals and a single unique internal orbital. In the two-dimensional planar polygonal systems (e.g., $C_5H_5^-$, C_6H_6, $C_7H_7^+$) the twin internal orbitals overlap pairwise to form the so-called σ-bonding network around the circumference of the polygon and the unique internal orbitals overlap cyclically to form the so-called π-bonding network. In the three-dimensional deltahedral systems (e.g., $B_nH_n^{2-}$, $C_2B_{n-2}H_n$) the twin internal orbitals overlap pairwise in the surface of the polyhedron and the unique internal orbitals form a multicenter core bond at the center of the polyhedron with the overlap corresponding to a K_n complete graph in which every vertex is connected by an edge to every other vertex.

The above bonding model for globally delocalized deltahedra makes the crude but convenient assumption that all pairwise overlaps of unique internal orbitals are the same despite different pairwise relationships such as the cis and trans relationships in an octahedron or the ortho, meta, and para relationships in an icosahedron. This assumption can be evaluated by comparison of the molecular orbital energies in octahedral $B_6H_6^{2-}$ obtained from this graph-theory derived model with those obtained from the 1962 LCAO-MO extended Hückel calculations of Hoffmann and Lipscomb.[11] In these calculations unlike later more sophisticated calculations the energies of pure core and surface molecular orbitals can be determined by removing the effects of mixing core

and surface molecular orbitals belonging to the same irreducible representation of the O_h point group of the octahedron. This analysis[12] indicates that the energies obtained from the Hoffmann–Lipscomb calculations[11] correspond to a ratio of 0.625 for the overlap of the unique internal orbitals of the _trans_ atom pairs relative to the _cis_ atom pairs as compared with a ratio of unity implied by an unweighted K_6 graph in the octahedral $B_6H_6^{2-}$. This level of agreement is more than sufficient for the simple graph–theory derived model to lead to the correct number of bonding orbitals and hence the correct number of skeletal electrons. A similar comparison of the above graph–theory derived bonding model and the Hoffmann–Lipscomb calculations[11] for icosahedral $B_{12}H_{12}^{2-}$ is considerably more complicated[12] but indicates that core–surface mixing of the corresponding T_{1u} orbitals is necessary for the two methods to agree at the level of giving the same number of skeletal bonding molecular orbitals.

The general approach for considering metal cluster bonding models involves calculating the number of available skeletal electrons for comparison with the number of skeletal electrons required to fill the bonding molecular orbitals for various cluster shapes and bonding topologies. If vertex atoms furnishing the normal three internal orbitals are considered, then BH, $Fe(CO)_3$, C_5H_5Co, and Pb vertices are examples of donors of two skeletal electrons and CH, $Co(CO)_3$, C_5H_5Ni, and Bi vertices are examples of donors of three skeletal electrons. Such relationships provide isoelectronic and isolobal[13] relationships between light atom and transition metal vertices leading, for example, to long recognized analogies[14] between polyhedral boranes and carboranes on the one hand and transition metal clusters on the other hand.

The globally delocalized deltahedra with n vertices (Figure 1) have $2n + 2$ skeletal electrons[15] with $2n$ of these electrons arising from the surface bonding and the remaining 2 electrons arising from the single molecular orbital generated by the

multicenter core bond.[2,10] Electron-rich polyhedra having more than $2n + 2$ apparent skeletal electrons have one or more non-triangular faces (Figure 2) whereas electron-poor deltahedra having less than $2n + 2$ apparent skeletal electrons have one or more tetrahedral chambers (Figure 3). If a deltahedron having $2n + 2$ skeletal electrons is regarded as topologically homeomorphic to a sphere, then a so-called _nido_ polyhedron having $2n + 4$ skeletal electrons is topologically homeomorphic to a sphere with a hole in it corresponding to the single non-triangular face.

The graph-theory derived method can also be used to derive reasonable electron-precise chemical bonding models for more complicated metal cluster structures. For example, globally delocalized rhodium octahedra can be fused by sharing triangular faces similar to the fusion of benzene rings by sharing edges (Figure 4).[8,9] Other rhodium carbonyl clusters have interstitial atoms which may contribute all of their valence electrons to the skeletal bonding. A prototypical example is $Rh_{13}(CO)_{24}H_2^{3-}$ (Figure 5) in which the volume requirement of the central interstitial Rh atom expands the outer Rh_{12} polyhedron from an icosahedron to a more voluminous cuboctahedron which however retains the globally delocalized bonding characteristic of icosahedral systems.[8,9] Platinum carbonyls form some unusual clusters (Figure 6) consisting of stacked triangles (e.g., $Pt_9(CO)_{18}^{2-}$) or stacked threaded pentagons (e.g., $Pt_{19}(CO)_{22}^{4-}$).[5,7] Electron-precise bonding models can be derived for these platinum clusters using edge-localized bonding in the platinum stack and delocalized bonding at each end of the platinum stack. The ends of the stacked triangles such as in $Pt_9(CO)_{18}^{2-}$ may be regarded as Möbius triangles[16] based on platinum d orbitals which change phase at each platinum atom.[5,7] The ends of the threaded pentagonal stack $Pt_{19}(CO)_{22}^{4-}$ may be regarded as _nido_ pentagonal pyramidal cavities electronically similar to the pentagonal pyramidal boron hydride B_6H_{10}.

Polyhedral Isomerizations

The role of polyhedra in the static description of chemical structures, including those of coordination compounds and metal clusters, makes the dynamic properties of polyhedra also of considerable interest. The central concept in the study of dynamic properties of polyhedra is that of a polyhedral isomerization, which may be defined as a deformation of a specific polyhedron P_1 until the vertices define a new polyhedron P_2. Of particular interest are sequences of two polyhedral isomerization steps $P_1 \rightarrow P_2 \rightarrow P_3$ in which the polyhedron P_3 is equivalent to the polyhedron P_1 but with some permutation of the vertices; such a polyhedral isomerization sequence is called a degenerate polyhedral isomerization with P_2 as the intermediate polyhedron. A degenerate polyhedral isomerization in which the intermediate P_2 is a planar polygon may be called a planar polyhedral isomerization.

Polyhedral isomerizations may be treated from either the microscopic or macroscopic points of view. The microscopic view uses the details of polyhedral topology to elucidate possible single polyhedral isomerization steps. The macroscopic view presents the relationships between different polyhedral isomers as graphs called topological representations in which the vertices depict different permutational isomers of a given polyhedron and the edges depict single degenerate polyhedral isomerization steps.[17] Typically the midpoints of the edges correspond to an intermediate polyhedron.

A necessary prerequisite to understanding the dynamics of polyhedra is the static topology of polyhedra. Of basic importance are relationships between possible numbers and types of vertices (v), edges (e), and faces (f) of polyhedra. Most fundamental is Euler's relationship

$$v - e + f = 2 \tag{4}$$

The edges may be related to the faces and vertices as follows where f_i and v_i refer to the number of faces with i edges and vertices of degree i, respectively:

$$\sum_{i=3}^{v-1} if_i = 2e \qquad (5a)$$

$$\sum_{i=3}^{v-1} iv_i = 2e \qquad (5b)$$

Since $f_i = v_i = 0$ for $i = 1$ and 2, the following inqualities must hold:

$$3f \leq 2e \qquad (6a)$$

$$3v \leq 2e \qquad (6b)$$

The equality holds for equation 6a in the case of deltahedra and for equation 6b in the case of polyhedra in which all vertices have degree 3.

In generating actual polyhedra the operations of <u>capping</u> and <u>dualization</u> are often important. Capping a polyhedron P_1 consists of adding a new vertex above the center of one of its faces F_1 followed by adding edges to connect the new vertex with each vertex of F_1 to give a new polyhedron P_2 having one more vertex than P_1 (Figure 7). A given polyhedron P can be converted into its dual P^* by locating the centers of the faces of P^* at the vertices of P and the vertices of P^* above the centers of the faces of P. Two vertices in the dual P^* are connected by an edge if and only if the corresponding faces in P share an edge. This process of dualization has the following properties:

(1)   The numbers of vertices and edges in a pair of dual polyhedra P and P^* satisfy the relationship $v^* = f$, $e^* = e$, $f^* = v$.

(2)   Dual polyhedra have the same symmetry elements and thus belong to the same symmetry point group.

(3)   Dualization of the dual of a polyhedron leads to the original polyhedron.

(4)   The degrees of the vertices of a polyhedron correspond to the number of edges in the corresponding face polygons of its dual.

(5). The duals of the cube, I_h dodecahedron, and n-prism are the octahedron, icosahedron, and n-bipyramid, respectively; the tetrahedron and n-pyramids are duals of themselves.

The problem of classification and enumeration of polyhedra is very complicated since there are no formulas, direct or recursive, for computing the numbers of combinatorially distinct polyhedra having given numbers of vertices, edges, and/or faces. Duijvestijn and Federico[18] have shown that there are 1, 2, 7, 34, 257, 2606, and 32300 topologically distinct polyhedra having 4, 5, 6, 7, 8, 9, and 10 faces or vertices, respectively, indicating that the number of topologically distinct polyhedra increases rapidly as the number of vertices or faces is increased. The detailed properties have been tabulated for all 301 topologically distinct polyhedra having 8 or fewer faces[19] or vertices[20]; these two tabulations,[19,20] of course, are equivalent by dualization (see above).

Now consider some microscopic aspects of polyhedral isomerizations. As early as 1966 Lipscomb[21] described framework rearrangements (isomerizations) in boranes and carboranes in terms of diamond-square-diamond (dsd) processes. Such a dsd process in a polyhedron occurs at two triangular faces sharing an edge and can be depicted as follows:
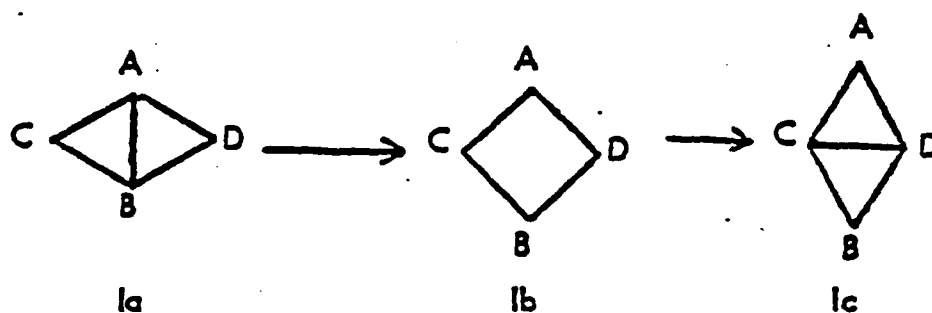
A configuration such as Ia can be called a <u>dsd situation</u>, the edge AB a <u>switching edge</u>, and the quadrilateral face ACBD in structure Ib a <u>pivot face</u>.[22] If a, b, c, and d are

the degrees of vertices A, B, C, and D, respectively, then the requirement for a degenerate dsd process is

$$c = a-1 \text{ and } d = b-1 \quad \text{ or } c = b-1 \text{ and } a = a-1 \qquad (7).$$

A deltahedron with e edges has e distinct dsd situations; if at least one of these dsd situations is degenerate by satisfying equation 7, then the deltahedron is inherently fluxional.[22] If none of the e distinct dsd situations of a deltahedron is degenerate by satisfying equation 7, then the deltahedron is inherently rigid. The inherent rigidity/fluxionality of deltahedra having various numbers of vertices (Figure 1) is summarized in Table 1; the chemical significance of this is summarized elsewhere.[22]

Now consider some macroscopic aspects of polyhedral isomerizations as depicted by topological representations,[17] which are graphs in which the vertices correspond to isomers and the edges correspond to isomerization steps. For isomerizations of a polyhedron with n vertices, the number of vertices in the topological representation is the isomer count I where

$$I = n!/|R| \qquad (8)$$

and $|R|$ is the number of proper rotations $(E + \text{all } C_k)$ in the symmetry point group of the polyhedron in question. The degree of a vertex corresponds to the number of new permutational isomers generated in a single isomerization step from the isomer represented by the vertex in question; this number δ is called the connectivity. For topologically different polyhedra depicted in the same topological representation, the isomer counts I and I' and connectivities δ and δ' must satisfy the so-called closure condition,[17] i.e.

$$I\delta = I'\delta' \qquad (9).$$

A simple illustration of these ideas is provided in the four-vertex system by the topological representation of the degenerate planar isomerization of a tetrahedron into its enantiomer through a square planar intermediate (Figure 8).[17] The isomer count for the tetrahedron, I_{tet}, is $4!/|T| = 24/12 = 2$ and the isomer count for the square, I_{sq}, is $4!/|D_4| = 24/8 = 3$. A topological representation of this process is a $K_{2,3}$ bipartite graph,

TABLE 1

INHERENT RIGIDITY/FLUXIONALITY OF DELTAHEDRA

Vertices	Deltahedron (Figure 1)	Inherently Rigid or Fluxional
4	Tetrahedron	Rigid
5	Trigonal bipyramid	Fluxional
6	Octahedron	Rigid
7	Pentagonal bipyramid/ Capped octahedron	ML_7—fluxional Boranes—rigid
8	Bisdisphenoid ("D_{2d}-dodecahedron")	Fluxional
9	Tricapped trigonal prism (D_{3h})	Fluxional
10	Bicapped square antiprism (D_{4d})	Rigid
11	$B_{11}H_{11}^{2-}$ polyhedron (C_{2v})	Fluxional
12	Icosahedron	Rigid

which is derived from the trigonal bipyramid by deletion of the three equatorial-equatorial edges (Figure 8). The two axial vertices correspond to the two tetrahedral isomers and the three equatorial vertices correspond to the three square planar isomers. The connectivities of the tetrahedral (δ_{tet}) and square planar (δ_{sq}) isomers are 3 and 2, respectively, in accord with the degrees of the corresponding vertices of the $K_{2,3}$ graph (Figure 8). Since $l_{tet}\delta_{tet} = l_{sq}\delta_{sq} = 6$, the closure condition (equation 9) is satisfied for this topological representation.

The topological representations of isomerizations of polyhedra having five or more vertices lead to some interesting graphs.[17] The 20-vertex Desargues-Levy graph (Figure 9, top) is a topological representation of isomerizations of the 20 trigonal bipyramid permutation isomers through the 30 square pyramid permutation isomer intermediates represented by the edge midpoints. If the 20 trigonal bipyramid permutation isomers are depicted as the corresponding 10 pairs of enantiomers, then the topological representation reduces to the Petersen's graph (Figure 9, bottom). A topological representation of six-vertex polyhedral isomerizations is a double group regular dodecahedron with a K_5 complete graph (i.e., a pentagon and a pentagram with all 5 vertices in common) in each of the 12 faces (Figure 10. The 30 edge midpoints of the dodecahedron correspond to the 30 octahedron permutation isomers and the $(12)(10) = 120$ edge midpoints of the 12 K_5 graphs on the dodecahedron faces correspond to the 120 trigonal prism intermediates in trigonal twist[17,23] (i.e., Bailar twist or Ray and Dutt twist triple dsd) isomerization processes.

In the cases of isomerizations of polyhedra having more than six vertices, the isomer counts (equation 8) are too large (e.g., $l_{cube} = 8!/|O| = 40320/24 = 1680$) for topological representations to be depicted graphically in a tractable manner. In the case of 8-vertex polyhedra a tractable graphical topological representation can be obtained by "hyperoctahedral restriction" since the 384-operation symmetry group of the four-dimensional cube (tesseract)

contains the symmetries of all of the eight-vertex polyhedra of actual or potential chemical significance including the ordinary cube as well as the hexagonal bipyramid, square antiprism, and bisdisphenoid ("D_{2d}-dodecahedron").[24] The hyperoctahedrally restricted isomerizations of these 4 eight-vertex polyhedra can be depicted by the topological representation in Figure 11, namely a $K_{4,4}$ bipartite graph having 8 hexagon vertices.[24] The midpoints of the 16 edges of the $K_{4,4}$ bipartite graph represent hexagonal bipyramid (D_{6h}) enantiomer pairs, the 8 centers of the 8 hexagons represent cube (O_h) enantiomer pairs, the 48 vertices of the 8 hexagons represent square antiprism (D_{4d}) enantiomer pairs, and the midpoints of the 48 edges of the 8 hexagons represent bisdisphenoid (D_{2d}) enantiomer pairs. Note that when considering polyhedra for eight-coordination, sp^3d^4 hybrids suffice to form square antiprisms and bisdisphenoids whereas hybrids containing f orbitals are required to form cubes and hexagonal bipyramids.[25] Thus eight-vertex isomerizations involving only s, p, and d orbitals are restricted to the circumference of a single hexagon where square antiprism and bisdisphenoid isomers are located whereas the availability of f orbitals as well as s, p, and d orbitals makes accessible the hexagon centers representing cubes as well as transitions between hexagons along the edges of the $K_{4,4}$ bipartite graph representing hexagonal bipyramids.

Conclusion

This short article illustrates how mathematical ideas taken from disciplines such as topology and graph theory can provide fundamental theoretical insight into key areas of coordination chemistry such as structure and bonding of metal clusters as well as polyhedral isomerizations. Such theoretical insight is most valuable in the planning of effective and efficient experimental programs in diverse areas of coordination chemistry, including work of potential practical importance relating to topics such as molecular catalysis, properties of solid state materials, and bioinorganic chemistry.

Acknowledgment

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Figure 1:   Some chemically significant deltahedra without tetrahedral chambers.

Figure 2:   Some chemically-significant polyhedra having one or two non-triangular faces.

Figure 3:   Examples of chemically significant deltahedra with tetrahedral chambers.

Figure 4:   Some analogies between the fusion of rhodium carbonyl octahedra by sharing triangular faces and the fusion of benzene rings by sharing edges.

Figure 5:   The centered cuboctahedron found in $Rh_{13}(CO)_{24}H_2^{3-}$ and related clusters.

Figure 6:   Examples of stacked triangle and stacked threaded pentagon platinum carbonyl clusters.

Figure 7:-   Formation of new polyhedra by capping triangular (top) or quadrilateral (bottom) faces of polyhedra.

Figure 8:   The bipartite $K_{2,3}$ topological representation of the degenerate planar isomerization of a tetrahedron (T_d) into its enantiomer through a square planar intermediate (D_{4h}).
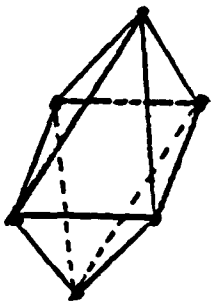
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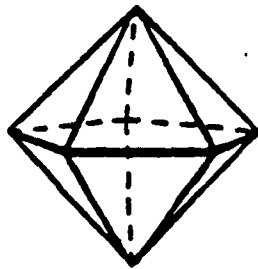
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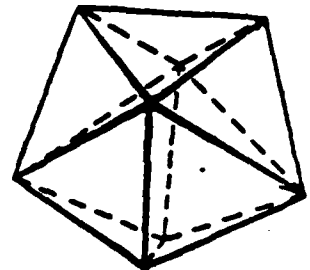
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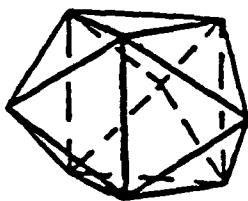
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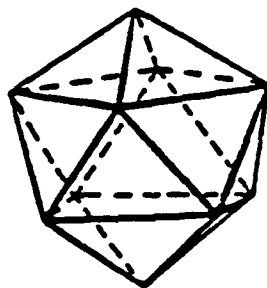
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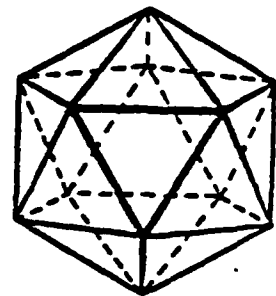
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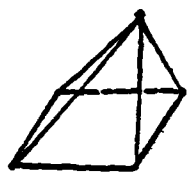
Square
Pyramid
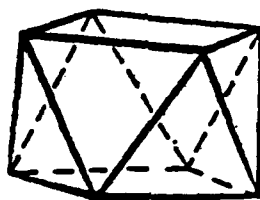
Square
Antiprism
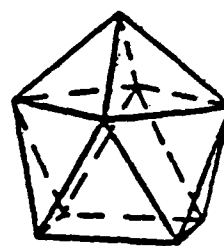
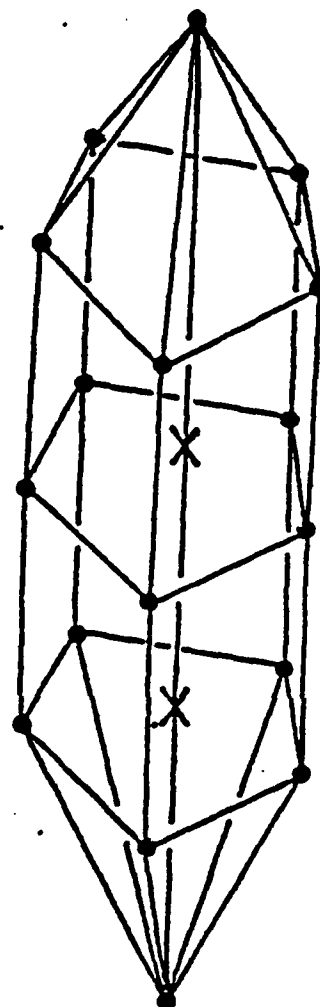Capped Square
Antiprism

Bicapped
Tetrahedron
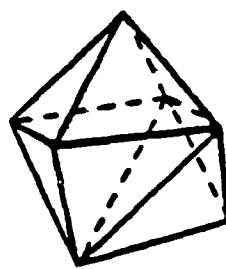
Capped
Octahedron
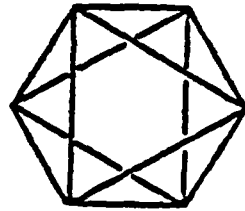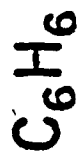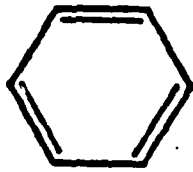
Benzene   Naphthalene   Anthracene   Perinaphthenide
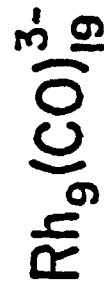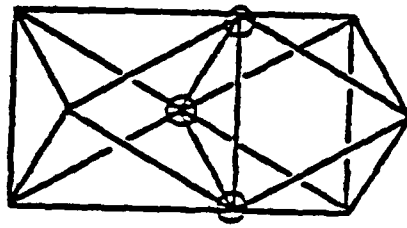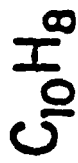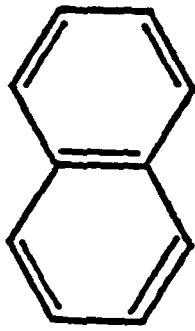
C_6H_6 $C_{10}H_8$ $C_{14}H_{10}$ $C_{13}H_9$

$Rh_6(CO)_{16}$ $Rh_9(CO)_{19}^{3-}$ $H_2Rh_{12}(CO)_{25}$ $Rh_{11}(CO)_{23}^{3-}$

interior
triangle

exterior
triangles

$Pt_9(CO)_{18}^{2-}$

$Pt_{19}(CO)_{22}^{4-}$
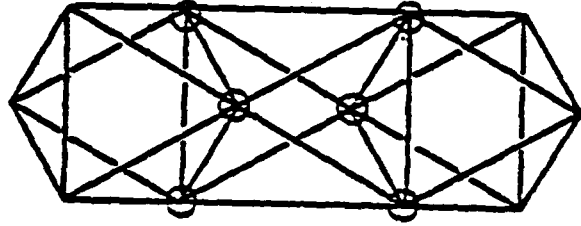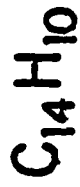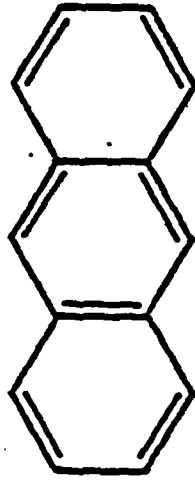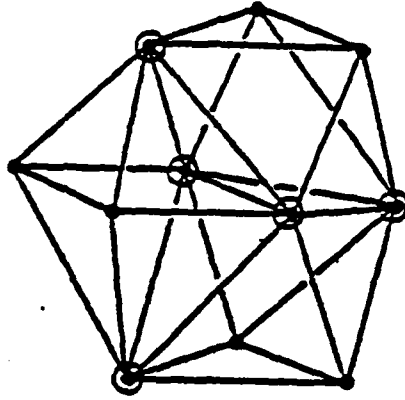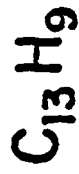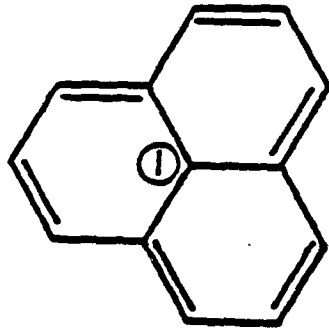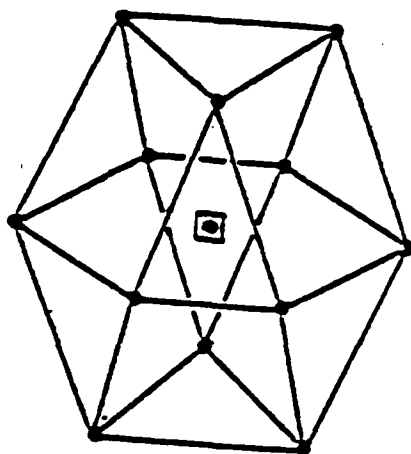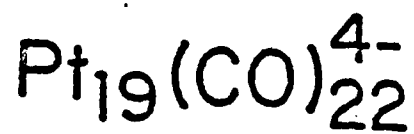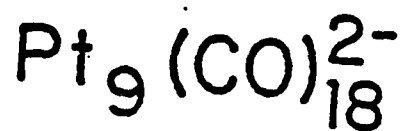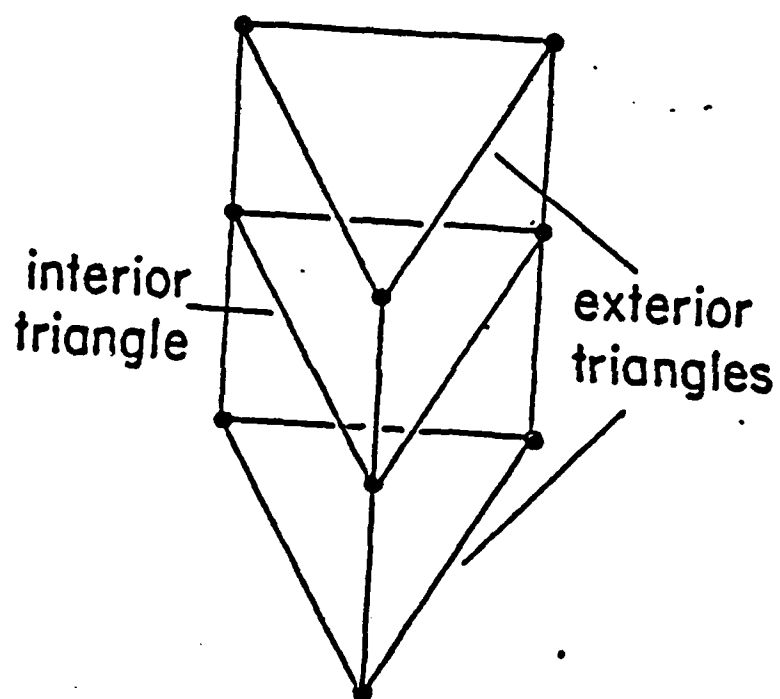
TRIANGULAR FACE
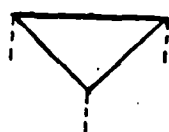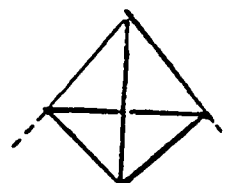
P_1 $\longrightarrow$ P_2

$v_2 = v_1 + 1$ $e_2 = e_1 + 3$ $f_2 = f_1 + 2$

QUADRILATERAL FACE
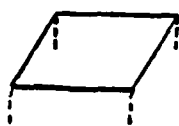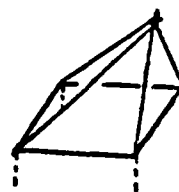
P_1 $\longrightarrow$ P_2
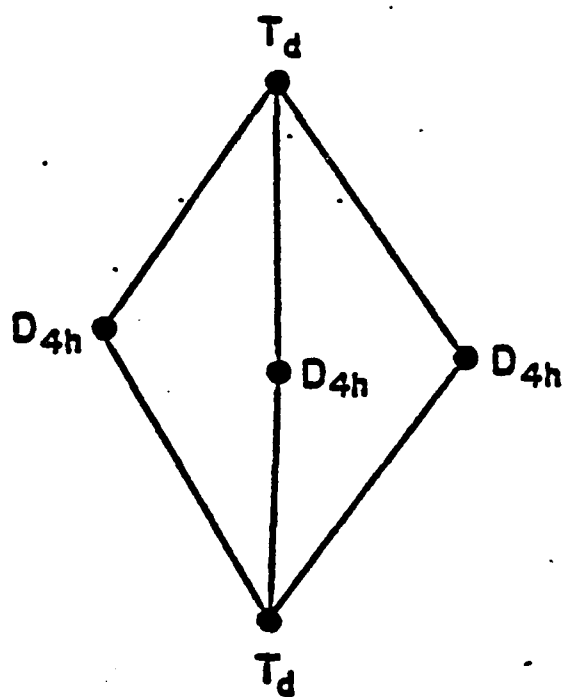
$v_2 = v_1 + 1$ $e_2 = e_1 + 4$ $f_2 = f_1 + 3$
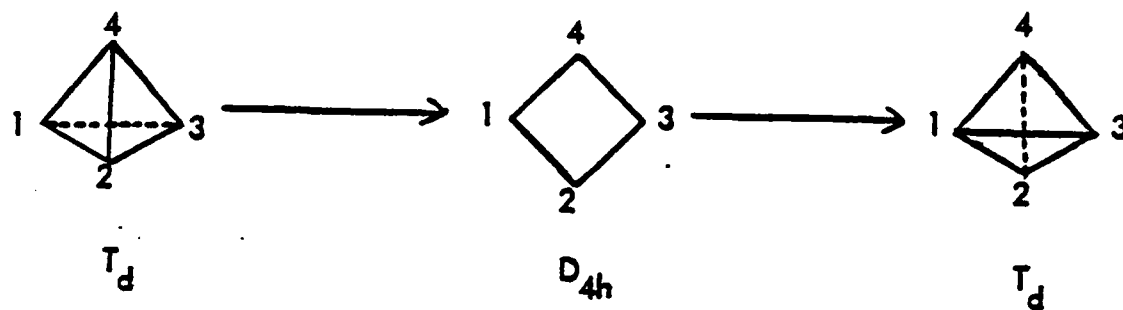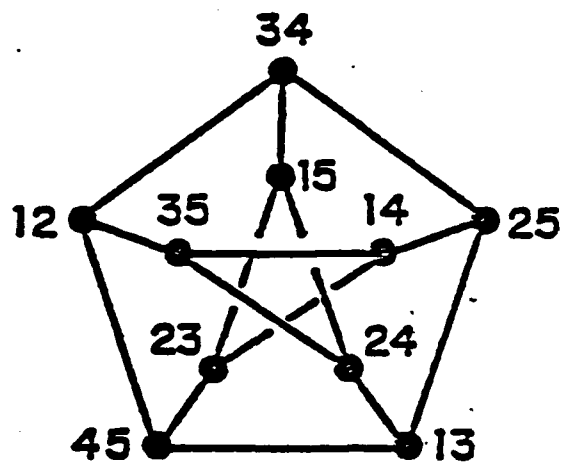
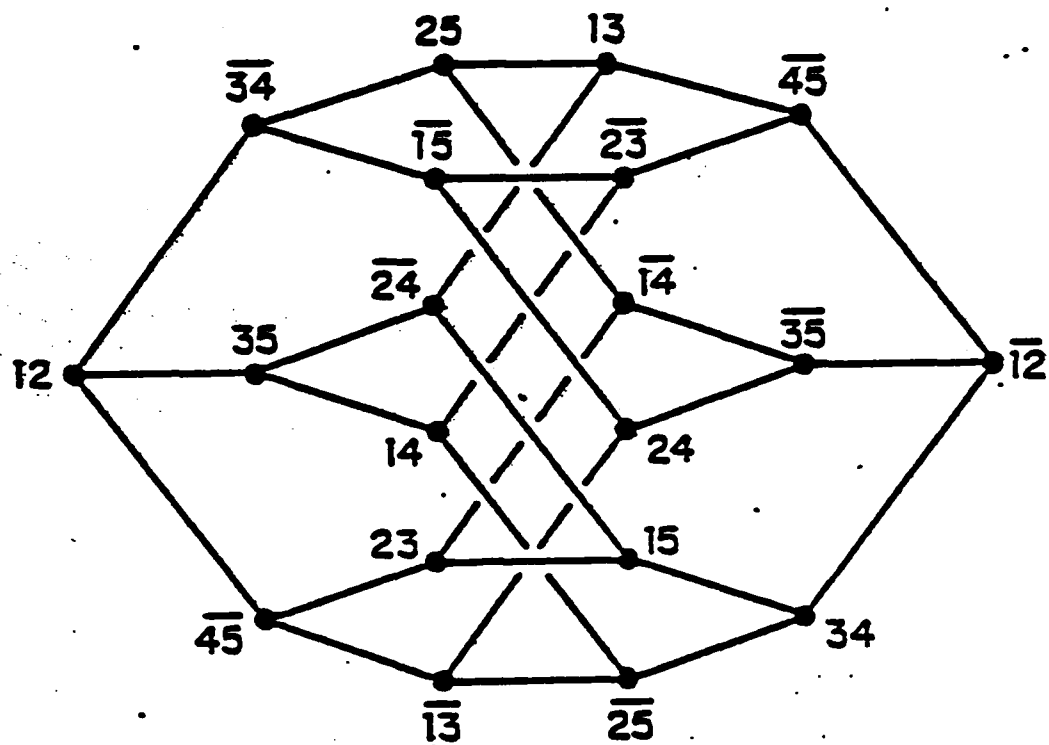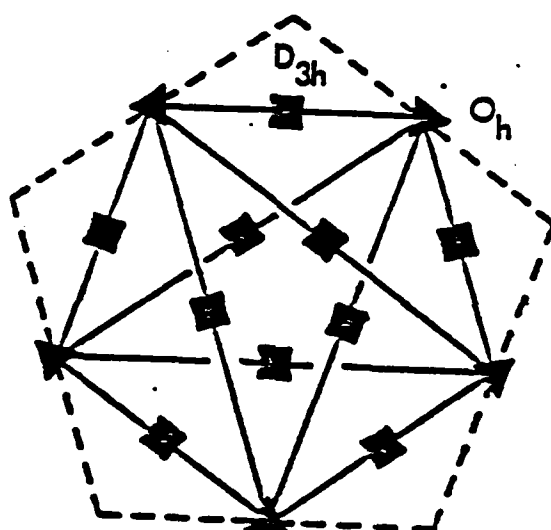$T_d \rightarrow D_{4h} \rightarrow T_d$

Figure 9: Top: the Desargues-Levy graph as a topological representation of the isomerizations of the 20 trigonal bipyramid permutation isomers (the vertices) through the 30 square pyramid permutation isomer intermediates (the edge midpoints). Bottom: the Petersen's graph as a topological representation of the isomerizations of the 10 trigonal bipyramid enantiomer pairs (the vertices) through the 15 square pyramid enantiomer pair intermediates (the edge midpoints). The trigonal bipyramid isomers are labelled by the ligands in the axial positions with bars being used to differentiate enantiomers.
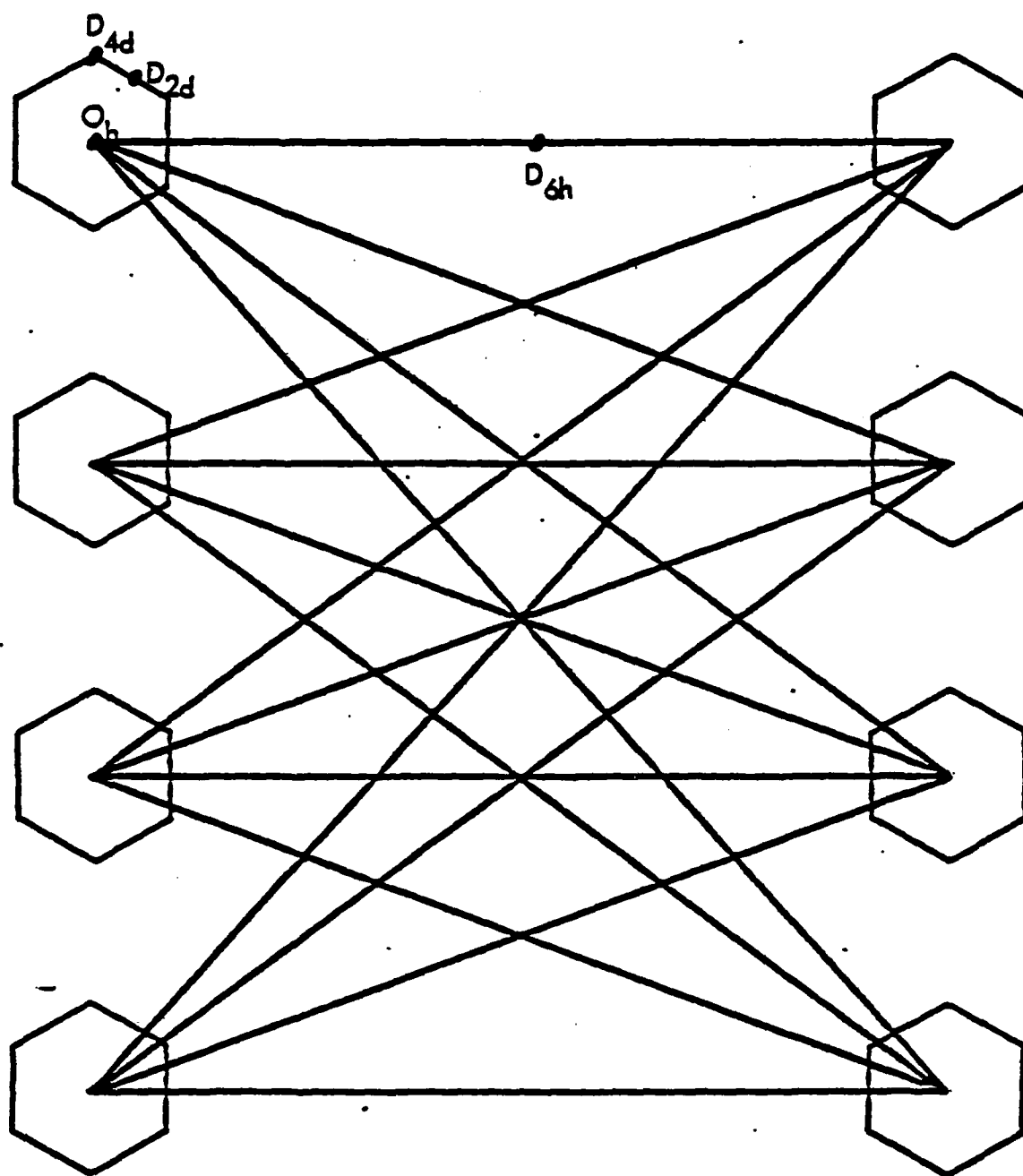
Figure 10: The K_5 complete graph on each of the 12 pentagonal faces of the double group pentagonal dodecahedron topological representation of the 30 octahedron permutation isomers (triangles) through the 120 trigonal prism intermediates (squares).

Figure 11: The $K_{4,4}$ bipartite graph of hexagons as a hyperoctahedrally restricted topological representation of isomerizations of eight-vertex polyhedra showing the locations of one of the eight cubes (O_h), 16 hexagonal bipyramids (D_{6h}), 48 square antiprisms (D_{4d}), and 48 bisdisphenoids (D_{2d}).

D_{4d}

D_{2d}

O_h

D_{6h}

END

1—81

DTIC